

# 2020 AFOSR Molecular Dynamics/Theoretical Chemistry Program Review

Dr. Michael Berman | May 19-21, 2020 | Virtually

## Agenda Day 1 | Tuesday, May 19, 2020

Time	Topic	Speaker
9:30	Sign-in	
10:00	Intro Remarks	
10:10	Probing and Manipulating the Photophysics of New Semiconducting Carbon Nanotube Films	Martin Zanni, Wisconsin
10:35	Fe and Ni Molecular Photochemistry Revealed by Femtosecond M-edge XANES	Josh Vura-Weis, Illinois
11:00	<b>BREAK</b>	
11:20	Modeling the Nanoscale Fluctuations of the Electric Double-layer	Adam Willard, MIT (MURI)
11:45	Control of the Selectivity of Alkane Dehydrogenation for Endothermic Cooling on Supported Pt Cluster Catalysts	Anastassi Alexandrova, UCLA
12:10	Vibrational Spectroscopy of Water at Graphene Electrode Surfaces	Stephen Cronin, USC
12:35	<b>LUNCH</b>	
1:45	Playing with the DOLFIN	Dmitri Talapin, Chicago
2:10	Making New Materials from Molecular and Superatomic Building Blocks	Colin Nuckolls, Columbia
2:35	Aluminum-based Bridged Superatomic Molecule: Unusual Nano p- n- junction with Tunable Band gap, Adjustable Band alignment, and Effective Electron Hole Separation	Shiv Khanna, VCU
3:00	<b>BREAK</b>	
3:20	DES and SILs: Improving Energetics by Applying Modern Concepts	Stefan Schneider, AFRL
3:45	Molecular Simulation of Solid Propellants: Models for Ammonium Perchlorate and Hydroxyl-Terminated Polybutadiene	Edward Maginn, Notre Dame
4:15	<b>MEETING ADJOURN</b>	

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## Agenda Day 2 | Wednesday, May 20, 2020

Time	Topic	Speaker
9:30	Sign-In	
10:00	Intro Remarks	
10:10	Plasmonic Photocatalysis with Antenna-Reactor Particles	Naomi Halas, Rice U (MURI)
10:35	Influencing the Nonlinear Optical and Electronic Properties of 2D Materials at the Atomic Level	Kenneth Knappenberger, Penn St.
11:00	Surface Plasmons for Inducing and Probing Surface Photochemistry	Terefe Habteyes, UNM
11:25	<b>BREAK</b>	
11:45	Trapped Hole Diffusion in Semiconductor Nanocrystals	Gordana Dukovic, Colorado
12:10	Probing the Electronic Structure of Ligand-Protected Metal Nanoclusters Using Atomically-Precise Spectroscopic Methods	Christopher Johnson, Stony Brook
12:35	Molecular Reaction Imaging of Charge Generation, Transport, and Recombination in Ultrathin 2D Semiconductors	Justin Sambur, Colorado St
1:00	<b>LUNCH</b>	
2:00		Berman, AFOSR
2:25	Break Out Rooms	
4:00	<b>MEETING ADJOURN</b>	

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## Agenda Day 3 | Thursday, May 21, 2020

Time	Topic	Speaker
9:30	Sign-in	
10:00	Intro Remarks	
10:10	Capture and Characterization of Small Molecules Activated by Homogeneous Catalysts using Cryogenic Ion Chemistry and Spectroscopy	Mark Johnson, Yale
10:35	Solvated Ion Cluster Dissociation Rates for Ionic Liquid Electrospray Propellants	Benjamin Prince, AFRL
11:00	Effects of Organic Moieties on the Optical Properties of Inorganic Frameworks	Ruth Pachter, AFRL
11:25	<b>BREAK</b>	
11:45	Vibrational Polaritons: Reactivity and Spectroscopy	Joel Yuen-Zhou, UCSD
12:10	Probing Carbon-Carbon Bond Breaking and Bond Formation as it Applies to Endothermic Fuels Development	Chris Bunker, AFRL
12:35	Watching Solids and Liquids through the Ultrafast Shock Compression Microscope	Dana Dlott, Illinois
1:00	<b>MEETING ENDS</b>	